

Pentane
109-66-0 | DTXSID2025846

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 35.6

Global applicability domain: Inside

Local applicability domain index: 6.14e-01

Confidence level: 7.27e-01

Nearest Neighbors from the Training Set

Image not found

Cyclohexane

Measured: 83.2

Predicted: 59.1

Image not found

Methylcyclohexane

Measured: 186

Predicted: 233

Image not found

Benzene

Measured: 4.27

Predicted: 10.0

Image not found

Quinoline

Measured: 3.80

Predicted: 6.66

Image not found

Dicyclopentadiene

Measured: 219

Predicted: 228